

STATISTICS OF DYNAMIC NETWORKS: A DEPTH FUNCTION APPROACH

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ABSTRACT. The study of random graphs and networks had an explosive development in the last couple of decades. Meanwhile, techniques for the statistical analysis of sequences of networks were less developed. In this paper we focus on networks sequences with a fixed number of labeled nodes and study some statistical problems in a nonparametric framework. We introduce natural notions of center and a depth function for networks that evolve in time. We develop several statistical techniques including testing, supervised and unsupervised classification, and some notions of principal component sets in the space of networks. Some examples and asymptotic results are given, as well as two real data examples.

1. INTRODUCTION

In the last fifteen years, applications of random networks have expanded beyond mathematics, physics, and computer science. Many climatologists, neuroscientists, biologists, sociologists, and economists are becoming more interested in the subject. Networks provide useful representations for many experimental and artificial phenomena.

A large number of research lines in random networks are developed each year. Most of these developments can be classified in one (or both) of the following two categories: probabilistic modeling or statistical analysis. In the former, the focus is on developing new models or deepen the knowledge of an existing model capable of reproducing some network properties. Some important results among these lines include the existence of stationary measures in dynamic models (Watts and Strogatz, 1998) or static but growing in size (Barabasi and Albert, 1999; Fraiman, 2008), characterizations of thresholds for giant components and connectivity (Bollobás et al., 2007; Devroye and Fraiman, 2014), and analysis of the spread of epidemics over fixed networks. In the latter category, the main goal is to develop mathematical tools for obtaining a precise characterization or description of real networks. Examples of this category include the development of modularity measures (Newman, 2006; Bickel and Chenb, 2009), network motifs, community detection (Newman and Girvan, 2004; Zhao et al., 2012, 2011), spectral network analysis (Rohe et al., 2011; Karrer and Newman, 2011) among others. Our contribution belong to this category of statistical characterization. The literature concentrates mostly on *individual* network analysis. However, we are rather interested in studying a *set* of networks. We propose a new way to describe, classify, perform principal components and test a *dependent sequence* of networks.

The statistical study of a sequence of networks has received little attention. A relevant reference in this direction is Kolar et al. (2010) where they estimate parametric time varying networks. One of the main interesting aspects of our proposal is that it is non-parametric. We discuss how some multivariate statistical methods can be adapted to analyze a random sample of networks or the stochastic dynamics of an evolving network.

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In many networks, such like those modeling brain connections, financial markets, the internet, or protein interactions, the label that identifies each node appears naturally and is relevant. For example, a node can represent a particular region of the brain with its own characteristics. Despite this fact the theory of random networks is dominated by models where node labels are not important for the kind of properties studied. In this work we consider the space of networks where each node is distinguishable. Specifically, we address the following questions:

- (a) Given a random network \mathbf{G} .
 1. How to define measures of centrality and variability?
 2. How to define a depth function in the space of networks?
- (b) Given a sample of networks G_1, G_2, \dots, G_ℓ .
 1. How to calculate their empirical measures of centrality and variability?
 2. How to perform hypothesis testing for the one and the two sample problem?
 3. How to define a notion of principal components?
 4. How to perform supervised and unsupervised classification?

This short list include several of the most commonly used techniques in applications in statistics. Our approach provides a way to deal with statistical problems using only the metric structure of the space where the random elements are defined.

We present some answers based on the definition of a depth function, which is defined by a distance in the space of networks, that has the nice property of determining the distribution of a random network. We develop some statistical analysis tools based on it, and show that many standard problems in multivariate analysis can be easily adapted to our framework.

One major issue when working with network data is the implementation of the proposed techniques for large scale networks. For all the problems addressed in the manuscript we find explicit algorithms which allow to implement our methods with a computational complexity of order n^2 (in fact, linear in the number of links), where n is the number of nodes, so we can deal with large scale networks and big datasets. We show several results regarding consistency and asymptotic distribution, and two real data applications. We also exhibit simple and explicit formulae to calculate depth, center and principal components. All proofs are given in the Appendix.

2. PROBABILITY AND GRAPH THEORY FRAMEWORK

A network, denoted by $G = (V, E)$, is described by a set V of nodes (vertices) and a set $E \subset V \times V$ of links (edges) between them. In what follows, we consider families of networks defined over the same fixed finite set of n nodes and $m = n(n-1)/2$ stands for the total number of possible links. Then, a network is completely described by its adjacency matrix $A \in \{0, 1\}^{n \times n}$, where $A_{ij} = 1$ if and only if the link $(i, j) \in E$.

2.1. Metrics on the space of networks. Several distances can be considered on the space of networks. The graph edit distance is one of the most flexible distance measures that have been proposed. For unlabeled networks, the graph edit distance between two networks is defined as the cost of the least expensive sequence of edit operations that are needed to make one network isomorphic to another one. The edit operations may include insertion, deletion or substitution of links and nodes. In general it is not easy to calculate this distance and several algorithms have been proposed to implemented. See for instance Gao et al. (2010) for a survey. However, in our setup, since the number of nodes n is fixed and nodes are labeled, it becomes much easier. In particular, the edit operations are reduced to insertion or deletion of a link, and no isomorphisms are considered.

Given two networks, G and H an edit path $\mathcal{T} = T_1 T_2 \cdots T_k$ between them is a sequence of edit operations that takes G into H . Let $\Gamma(G, H)$ the set of edit paths between G and H . A cost is given to each edit operation, $c(T_i)$, representing whether or not the edit operation is a strong modification of the network. Then, the edit distance is defined as

$$d(G, H) = \min_{\mathcal{T} \in \Gamma(G, H)} \sum_{i=1}^k c(T_i).$$

If the cost of adding or deleting a given link is the same, the edit operations are flips T_{ij} of the link (i, j) , which exchanges 1 with 0 on the (i, j) entry of the adjacency matrix of the network, and the costs can be assigned to the links. In this case

$$(1) \quad d(G, H) = \sum_{i < j} |A_{ij} - B_{ij}| c_{ij} = \sum_{A_{ij} \neq B_{ij}} c_{ij},$$

where c_{ij} is the cost of adding or deleting the link (i, j) , and A, B are the adjacency matrices of the networks G and H respectively. In particular, if all the costs are equal to 1, then it is just the L^1 distance between the adjacency matrices A and B . In order for d to be a distance, we assume that all costs $c_{ij} > 0$. In what follows, the space of networks with n nodes endowed with the metric (1) is denoted by \mathcal{G} .

Another interesting distance, but computationally very expensive, have been recently introduced by Pignolet et al. (2015) that takes into account the order in which the edit operations are executed. More precisely, the distance is defined as follows. Consider the subset of pairs of networks $\mathcal{M} \subset \mathcal{G} \times \mathcal{G}$ of the form $(G, T(G))$, i.e., those which can be converted into each other with only one graph edit operation. To each pair $(G, T(G)) \in \mathcal{M}$ assign a cost, given by $c : \mathcal{M} \rightarrow \mathbb{R}^+$. Then, the distance is defined as

$$d(G, H) = \min_{\mathcal{T} \in \Gamma(G, H)} \sum_{i=0}^{k-1} c(\mathcal{T}_i(G), \mathcal{T}_{i+1}(G)),$$

where $\mathcal{T}_0(G) = G$ and $\mathcal{T}_i = T_1 \cdots T_i$. The inconvenience of this distance is that the number of costs that must be known is $\#\mathcal{M} = m2^m$. For this reason, it is important in this case to have an explicit formula for c , but in general it is not clear what would be adequate for real network data.

All the results that follow can be developed using any distance between networks. However, we work with the edit distance (1) for which we obtain explicit algorithms of low computational cost (of order n^2) to develop the statistical problems addressed.

2.2. Centers, and scale measure. The notions of center and variability around it are fundamental to describe the distribution of a set of networks. Given that we have a metric in the space of networks there is a simple way to define them. In what follows we describe how to calculate this two important summarizing quantities.

We use boldface typeface for random elements. Let $p_G = \mathbb{P}(\mathbf{G} = G)$. The expected distance from a network H to a random network \mathbf{G} can be computed as

$$\mathbb{E}(d(\mathbf{G}, H)) = \sum_{G \in \mathcal{G}} d(G, H) p_G.$$

Definition 1. The *central (or median) set* \mathcal{C} of a random network \mathbf{G} is the Frechet center with respect to the metric d , that is the subset of networks

$$(2) \quad \mathcal{C} := \arg \min_{H \in \mathcal{G}} \mathbb{E}(d(\mathbf{G}, H)).$$

The notion of median subset corresponds to minimizing the expected L^1 -distance. A notion of mean subset can be defined by minimizing the expected L^2 -distance. In the Euclidean setup they correspond to the L^1 -median and to the usual expected value respectively. Given a sample G_1, \dots, G_ℓ of random networks in \mathcal{G} , applying definition (2) to the empirical distribution, the notion of empirical center is obtained. More precisely,

Definition 2. The *empirical central set* $\hat{\mathcal{C}}_\ell$ is defined as the subset of networks fulfilling

$$(3) \quad \hat{\mathcal{C}}_\ell = \arg \min_{H \in \mathcal{G}} \frac{1}{\ell} \sum_{i=1}^{\ell} d(G_i, H).$$

In general, the sets \mathcal{C} and $\hat{\mathcal{C}}_\ell$ contain only one network, i.e., there exists a unique network that minimizes equations (2) and (3) respectively. In this case, we call the unique central network the *skeleton network* and we denote it by S (or \hat{S}_ℓ in the empirical case). Note that in contrast to what is usually called the empirical average network (the sum of the adjacency matrices divided the number of networks) the skeleton belongs to the space of networks.

The following proposition gives necessary and sufficient conditions for uniqueness of the central network, together with a complete characterization of the skeleton network and the subsets $\mathcal{C}, \hat{\mathcal{C}}_\ell$ when we have more than one solution. In the last case, the elements of the set form a lattice and there is a network in \mathcal{C} (respectively in $\hat{\mathcal{C}}_\ell$) with the minimum number of links and another one with the maximum number of links. These are called the minimal and maximal centers respectively.

Proposition 1 (Characterization of the central set).

- a) \mathcal{C} has a unique network if and only if $\mathbb{P}(\mathbf{A}_{ij} = 1) \neq 1/2 \ \forall i, j$. The adjacency matrix of $S(\mathbf{G})$ satisfies $A_{ij}^S = 1$ if and only if $\mathbb{P}(\mathbf{A}_{ij} = 1) > 1/2$.
- b) $\hat{\mathcal{C}}_\ell$ has a unique network if and only if $(1/\ell) \sum_{k=1}^{\ell} A_k(i, j) \neq 1/2 \ \forall i, j$. The adjacency matrix of \hat{S}_ℓ satisfies $A_{ij}^S = 1$ if and only if $(1/\ell) \sum_{k=1}^{\ell} A_k(i, j) > 1/2$.
- c) Otherwise, for some pair (i, j) we have $\mathbb{P}(\mathbf{A}_{ij} = 1) = 1/2$. Define the minimal and maximal centers, S and L , to be the networks whose adjacency matrices respectively satisfy that $A_{ij}^S = 1$ if and only if $\mathbb{P}(\mathbf{A}_{ij} = 1) > 1/2$, and $A_{ij}^L = 1$ if and only if $\mathbb{P}(\mathbf{A}_{ij} = 1) \geq 1/2$. Then, the set \mathcal{C} contains exactly all subnetworks of L for which S is a subnetwork. The same is true for the empirical version *mutatis mutandis*.

The relevance of this last result is that it avoids finding the minimum by exhaustive search. If the empirical central network is unique then it contains only the links that are observed more than half of the time. Moreover, since the space of networks \mathcal{G} is finite, the law of large numbers follows immediately.

Theorem 1. Let \mathbf{G} be a random network with law μ such that the central set \mathcal{C} has only one element S . Let $\{\mathbf{G}_t, t \geq 1\}$ be an stationary and ergodic sequence of random networks with law μ . If \hat{S}_ℓ is any element of the empirical central set $\hat{\mathcal{C}}_\ell$, then almost surely

$$\lim_{\ell \rightarrow \infty} d(S, \hat{S}_\ell) = 0.$$

In other words, the set of empiric central networks coincides with the skeleton network if ℓ is large enough. In general, if the central set \mathcal{C} has more than one element, we have that $\hat{S}_\ell \in \mathcal{C}$.

We are interested in a measure of the “homogeneity” (variability) of a random network. The most natural notion of dispersion associated with our problem is the following.

Definition 3. Let $S^* \in \mathcal{C}$. The *scale* of the random network \mathbf{G} is defined as

$$\sigma := \mathbb{E}(d(\mathbf{G}, S^*)).$$

The corresponding empirical scale measure $\hat{\sigma}_\ell$ based on the sample G_1, \dots, G_ℓ , is obtained by replacing the expected distance by $(1/\ell) \sum_{i=1}^\ell d(G_i, S^*)$ in Definition 3. We can derive strong consistency of $\hat{\sigma}_\ell$ to σ from Theorem 1, using the inequality

$$\frac{1}{\ell} \sum_{i=1}^\ell |d(G_i, \hat{S}_\ell) - d(G_i, S)| \leq \max_{H \in \mathcal{G}} |d(H, \hat{S}_\ell) - d(H, S)|.$$

We finish this section presenting two examples to illustrate the proposed framework.

Example 1. An important distribution that arises in the space of networks \mathcal{G} is the (double) exponential type distribution given by

$$(4) \quad \mathbb{P}(\mathbf{G} = H) = ze^{-\lambda d(H, S_0)}.$$

If all costs are equal, the normalizing constant $z = e^{\lambda m}(1 + e^\lambda)^{-m}$, $\lambda > 0$ is a parameter, and S_0 is a particular network. As in the real double exponential distribution, this law is symmetric, it has an explicit symmetry center and mode (S_0), and has an exponential decay. It is a particular case of the so called Exponential Random Graph Model, and presents a unique central network (2). It is easy to show that it verifies $S = S_0$, and $\sigma = m/(1 + e^\lambda)$.

Note that the empirical center given in (3) can be seen as a *maximum likelihood* estimate of the center of the previous distribution. Indeed, if G_1, \dots, G_ℓ are i.i.d. random networks with this μ distribution, the empirical center coincides with the maximum likelihood estimate of S_0 .

Example 2. In the Erdős–Rényi model each link is present with a fixed probability p , independently. Unlike the previous example, the well known Erdős–Rényi model does not favor the presence of any link (nor a group of links), it is an homogeneous model. All networks with k links are equally likely in the sense that they have the same probability. If $p < 1/2$ the network is sparse. On the contrary, if $p > 1/2$ there exists a giant component, while $p = 1/2$ is the critical value. Our notion of center captures the homogeneity and symmetry of the model, and provides a natural notion of center. The central network is the empty network G_\emptyset (the network with no links) if $p < 1/2$, in the case $p > 1/2$ it is the complete network \mathbf{G}_Ω , and if $p = 1/2$ we get the entire space of networks.

For this model, the scale is $\sigma = (1/2 - |p - 1/2|)m$ which has its maximum at $p = 1/2$, and it is zero for p equal 0 and 1. This result is intuitive since the entropy is maximum at this value.

Remark 1. A different empirical notion of center has been introduced in Jiang et al. (2001), assuming that all costs are equal. It restricts the search of the minimizer to the networks in the sample, i.e., the center \hat{M}_ℓ is $\arg \min_j (1/\ell) \sum_{i=1}^\ell d(G_i, G_j)$. The population version corresponds to minimizing the expected distance over the support of the underlying distribution μ of \mathbf{G} , that is the center is defined as $\arg \min_{H \in \text{supp}(\mu)} \mathbb{E}(d(\mathbf{G}, H))$. If the support of μ is the whole space of networks \mathcal{G} both notions coincide. However, like in the case of high dimensional data, maximizing just over the sample, is not a good strategy. Indeed, for example, it is easy to verify (using Hoeffding's inequality) that for the

Erdős–Rényi model with parameter $p < 1/2$,

$$\begin{aligned}\mathbb{P}(\hat{S}_\ell \neq G_\emptyset) &\leq 1 - \left(1 - e^{-2\ell(p-1/2)^2}\right)^m, \\ \mathbb{P}(\hat{M}_\ell \neq G_\emptyset) &\geq \prod_{i=1}^{\ell} \mathbb{P}(\mathbf{G}_i \neq G_\emptyset) = (1 - (1-p)^m)^\ell.\end{aligned}$$

Thus, \hat{S}_ℓ converges at a much better rate.

3. DEPTH FUNCTION

In this section we first introduce a notion of depth in the space of networks. A depth function is a function that orders the space in terms of center-outward position. The idea has been introduced in the robust statistics literature. The most well known depth notions for the Euclidean space are the half-space depth (Tukey, 1975), simplicial depth (Liu, 1988), the L^1 -depth (Brown, 1983; Small, 1996) and Mahalanobis depth (Mahalanobis, 1936). Several important applications to different statistical problems based on depth concepts have been developed in the last years.

Given a fixed network H and a sample of random networks G_1, \dots, G_ℓ with the same distribution we consider the L^1 -depth notion with respect to the metric d , which in particular defines the central network (also called spatial median) in our setup. The central set corresponds with the set where this depth is maximized. More precisely,

Definition 4. We define the empirical depth at the network $H \in \mathcal{G}$, as

$$\hat{D}_\ell(H) = m - \frac{1}{\ell} \sum_{t=1}^{\ell} d(G_t, H),$$

which corresponds to the population depth given by $D(H) = m - \mathbb{E}(d(\mathbf{G}, H))$.

Observe that both the empirical and population depth are non-negative, and fulfill the main properties of a depth function given in Zuo and Serfling (2000). Moreover, we have a simple explicit solution for the median center maximizing $D(H)$ given by Proposition 1. On the contrary in the Euclidean space, an optimization method is required to maximize the L^1 -depth. In fact, a fast monotonically convergent algorithm to calculate the L^1 -median of a data set in \mathbb{R}^d has been proposed in Vardi and Zhang (2000).

An important property of Definition 4 is that the depth function determines the network law. This result, that follows from the invertibility of distance matrices given by Auer (1995), has an important impact in statistics and in particular in our setup since it allows to develop statistical methods based on the depth D and obtain results for the space of networks \mathcal{G} .

Proposition 2. *Given two distributions μ, ν on \mathcal{G} . Write $D_\mu(H) = m - E_\mu(d(\mathbf{G}, H))$ to explicitly note the dependency. Then, $\mu = \nu$ if and only if $D_\mu(H) = D_\nu(H)$ for all $H \in \mathcal{G}$.*

In general, depths do not determine distribution, the only known result is for Tukey's half space depth when the measure is discrete and can be found in Cuesta-Albertos and Nieto-Reyes (2008). The empirical depth function $\hat{D}(H)$ converges almost surely to the population version $D(H)$ uniformly. Indeed, as a consequence of the ergodic theorem we have the following theorem.

Theorem 2 (Uniform convergence of the depth function). *Given a stationary ergodic sequence of random networks $\{\mathbf{G}_t : t \geq 1\}$ with common law μ . Then, almost surely as $\ell \rightarrow \infty$, $\max_{H \in \mathcal{G}} |\hat{D}_\ell(H) - D_\mu(H)| \rightarrow 0$.*

Moreover, the asymptotic distribution of the depth process is Gaussian.

Theorem 3 (Asymptotic normality of the depth process). *Given a strictly stationary α -mixing sequence of networks $\{\mathbf{G}_t : t \geq 1\}$ in \mathcal{G} with common distribution μ fulfilling $\sum_{n=1}^{\infty} \alpha(n) < \infty$. Fix an ordering $(G_j)_{j=1, \dots, 2^m}$ of the elements of the space \mathcal{G} and define*

$$\mathbf{Z}_\ell = (\hat{D}_\ell(G_j) - D_\mu(G_j))_{j=1, \dots, 2^m}, \quad \mathbf{Y}_k = (d(\mathbf{G}_k, G_j) - \mathbb{E}(d(\mathbf{G}_k, G_j)))_{j=1, \dots, 2^m}.$$

If in addition $\sum_{k=1}^{\infty} \beta_0^T \mathbb{E}(\mathbf{Y}_1^T \mathbf{Y}_k) \beta_0 > 0$, for all β_0 with $\|\beta_0\| = 1$, then, $\sqrt{\ell} \beta_0^T \mathbf{Z}_\ell$ converges weakly as $\ell \rightarrow \infty$ to a normal distribution with mean zero and with the same variance as $\beta_0^T \mathbf{Y}_1$.

4. HYPOTHESIS TESTING: TEST BASED ON RANDOM PROJECTIONS.

In this section we study the one and two samples hypothesis testing problem. Here we are interested in comparing for example two samples of networks and determine if they belong to the same population. A naive approach is to test directly the two distributions (or their corresponding depths, see Proposition 2) with a Chi-square or a Kolmogorov type test based on the statistic $\max_{H \in \mathcal{G}} |\hat{D}_\ell(H) - D_\mu(H)|$. However, the computational cost is of order 2^m and it requires a huge sample size in order to have a large power. On the other side, tests based on random projections for the one and two samples problems, as those considered in Cuesta-Albertos et al. (2006, 2007), can be implemented in our setup since the space of networks $\mathcal{G} = \{0, 1\}^m$ is contained in \mathbb{R}^m . They are based on the use of Corollary 3.2 in Cuesta-Albertos et al. (2007), which we describe briefly. Let μ be a Borel probability measure on \mathbb{R}^m ($m \geq 2$). Given a direction $h \in \mathbb{R}^m$, let $\langle h \rangle$ be the one-dimensional subspace spanned by h and $\mu_{\langle h \rangle}$ the distribution of the orthogonal projection of \mathbb{R}^m onto $\langle h \rangle$, i.e., $\mu_{\langle h \rangle}(B) = \mu(\pi_{\langle h \rangle}^{-1}(B))$, for Borel $B \subset \mathbb{R}$.

Proposition 3 (Cuesta-Albertos et al., 2007, Corollary 3.2). *Let μ, ν be Borel probability measures on \mathbb{R}^m , where $m \geq 2$. Then $\mu = \nu$ if*

- a) *the absolute moments $M_n = \int \|x\|^n x d\mu(x)$ are finite and satisfy the Carleman condition $\sum_{n \geq 1} M_n^{-1/n} = \infty$,*
- b) *the set $\mathcal{E}(\mu, \nu) = \{h \in \mathbb{R}^m : \mu_{\langle h \rangle} = \nu_{\langle h \rangle}\}$, has positive Lebesgue measure.*

It is clear that any distribution in \mathbb{R}^m supported on $\{0, 1\}^m$ fulfills Carleman condition and the previous result holds. For statistical purposes this means that in order to address the one sample problem $H_0 : \mu = \mu_0$ vs $H_A : \mu \neq \mu_0$, or the two samples problem $H_0 : \mu = \nu$ vs $H_A : \mu \neq \nu$, where μ, μ_0 , and ν are distributions in the space of networks, a standard one dimensional test is enough. For example, a Kolmogorov–Smirnov test based on the projected data onto one randomly chosen (for instance uniformly on the unit sphere) is able to test the null hypothesis presented above (see Cuesta-Albertos et al., 2006, for more details).

To improve the power, we may use many random projections onto i.i.d. uniformly distributed directions h_1, \dots, h_q . For the two samples the procedure is as follows (the one sample problem is completely analogous).

Given two independent stationary and ergodic sequences of networks $\mathcal{G}_1 = \{\mathbf{G}_1^1, \dots, \mathbf{G}_{\ell_1}^1\}$, $\mathcal{G}_2 = \{\mathbf{G}_1^2, \dots, \mathbf{G}_{\ell_2}^2\}$ and q random directions $\{\mathbf{h}_1, \dots, \mathbf{h}_q\}$ on \mathbb{R}^m , define for each $i = 1, \dots, q$

$$\mathbf{X}_{ij} = \langle \mathbf{h}_i, \mathbf{G}_j^1 \rangle, \quad j = 1, \dots, \ell_1; \quad \mathbf{Y}_{ij} = \langle \mathbf{h}_i, \mathbf{G}_j^2 \rangle, \quad j = 1, \dots, \ell_2.$$

For each i consider the samples $\{\mathbf{X}_{ij} : j = 1, \dots, \ell_1\}$, $\{\mathbf{Y}_{ij} : j = 1, \dots, \ell_2\}$ and define the binary random variable \mathbf{Z}_i taking value one if the two samples Kolmogorov–Smirnov test of level

α reject the null hypothesis and zero otherwise. Let $\mathbf{Z} = \sum_{i=1}^q \mathbf{Z}_i$. Under the null assumption, \mathbf{Z} has a Binomial(q, α). Therefore, the exact p -value $= \mathbb{P}(\mathbf{Z} > a)$ can be computed.

5. SPARSE PRINCIPAL COMPONENTS

Principal components is an important statistical tool when analyzing data, particularly for high dimensional and functional data. The objective of this technique is to reduce the dimension p of the data using linear combinations of the variables. This is done by projecting the data onto the $k \ll p$ dimensional subspace which minimize the distance to the original random vector. Equivalently, the principal components can be defined iteratively. The first is the direction on which the projection of the random element has maximal variance. The next one, maximizes the variance of the projection on the orthogonal subspace to the first one and so on. The absence of projections in metric spaces makes the extension non trivial. Since the space of networks is very large we want a sparse notion of principal components. In what follows we introduce some methods in such direction for random elements in the space \mathcal{G} .

Let G_\emptyset be the empty network and write $|H| = d(H, G_\emptyset)$ for the sum of the costs of links in H . Given $G, H \in \mathcal{G}$ define the intersection network $G \wedge H$ as the network with only the common links to both. Note that $|G \wedge H|$ is the weighted inner product, given by the costs, between the adjacency matrices of G and H . Recall that, given a, b, x arbitrary points in a metric space, we say that x belongs to a geodesic from a to b if $d(a, b) = d(a, x) + d(x, b)$. So, if $d(G, H) = k$ then there are $k!$ geodesics between them. Given a network H we define the set $\mathcal{S}(H)$ of all geodesics curves in the space \mathcal{G} joining H with the complete network, denoted by G_Ω . In other words, $\mathcal{S}(H)$ is the set of all networks which have H as a subnetwork.

Given a random network \mathbf{G} , we define the first *principal component* as the set of networks \mathcal{Q}_1 that maximize the variance of the following “projection”

$$(5) \quad \mathcal{Q}_1 = \arg \max_{Q \in \mathcal{G}} \text{var} \left(\frac{|G \wedge Q|}{|Q|} \right).$$

If $\mathcal{Q}_1 = \{Q_1, \dots, Q_p\}$ then the *principal component space* is $\mathcal{S}_1 = \cup_{i=1}^p \mathcal{S}(Q_i)$. Typically the set \mathcal{Q}_1 is a single network. The analogue of having more than one network in \mathcal{Q}_1 in the classical Euclidean case is having eigenvalues of the covariance matrix with multiplicity greater than one.

To define the *second principal component* \mathcal{Q}_2 we consider the same problem, but now we maximize the variance within the “orthogonal” subset $\mathcal{G} \setminus \mathcal{S}_1$.

Observe that $H \in \mathcal{G} \setminus \mathcal{S}_1$ iff H has no links in common with any element in \mathcal{Q}_1 , i.e., it has no link in common with the network $\tilde{Q}_1 := Q_1 \vee \dots \vee Q_p$, which contains all links present in at least one Q_j , $j = 1, \dots, p$. In this sense we refer to $\mathcal{G} \setminus \mathcal{S}_1$ as the orthogonal subset. This particular network, \tilde{Q}_1 , can be considered as the most informative network to visualize \mathcal{S}_1 . The set $\mathcal{G} \setminus \mathcal{S}_1$ has cardinality $2^{m-|\tilde{Q}_1|}$. The next principal components are defined analogously. To define the corresponding empirical version of (5) let

$$\Delta_\ell(Q) = \frac{1}{\ell} \sum_{k=1}^{\ell} \frac{(|G_k \wedge Q| - \Lambda_\ell(Q))^2}{|Q|^2},$$

where $\Lambda_\ell(Q) = (1/\ell) \sum_{k=1}^{\ell} |G_k \wedge Q|$. The empirical principal component is

$$\hat{\mathcal{Q}}_1 = \{Q \in \mathcal{G} : \Delta_\ell^{\max} - \Delta_\ell(Q) < \varepsilon_\ell\},$$

where $\Delta_\ell^{\max} = \max_{Q \in \mathcal{G}} \Delta_\ell(Q)$ and $\varepsilon_\ell \rightarrow 0$.

Proposition 4 (Characterization of the sparse principal component sets). *Let E_{ij} be the network consisting of only the (i, j) link and $p_{ij} = \mathbb{P}(\mathbf{A}_{ij} = 1)$. If*

$$M_1 = \{(i, j) : 1 \leq i < j \leq n\} \quad \text{and} \quad L_1 = \arg \min_{(i, j) \in M_1} |p_{ij} - 1/2|,$$

then $\mathcal{S}_1 = \cup_{(i, j) \in L_1} \mathcal{S}(E_{ij})$. Analogously, if

$$M_k = \{(i, j) : A_{ij}^H = 0 \ \forall H \in \cup_{i=1}^k \mathcal{S}_i\} \quad \text{and} \quad L_k = \arg \min_{(i, j) \in M_k} |p_{ij} - 1/2|,$$

then $\mathcal{S}_k = \cup_{(i, j) \in L_k} \mathcal{S}(E_{ij})$.

Based on the previous proposition, a simple algorithm of order n^2 is presented below.

- **Step 1:** Compute $W(Q_i) := |\text{var}(|\mathbf{G} \wedge Q_i|/|Q_i|) - 1/2|$ for all Q_i with a single link.
- **Step 2:** Let $W(Q_{(1)}) \geq \dots \geq W(Q_{(M)})$ be the order statistics.
- **Step 3:** If there are no ties, the first principal space is the set of networks with $Q_{(1)}$ as a subnetwork, the second one is the set of networks for which $Q_{(2)}$ is a subnetwork and $Q_{(1)}$ is not, and so on. If there are ties, say for instance $W(Q_{(j_1)}) = W(Q_{(j_p)})$, the principal space is just the union of the principal spaces of each $Q_{(j_r)}$, for $r = 1, \dots, p$.

Remark 2. *Our definition of sparse principal components normalize the data by $|Q|$. The same normalization is used when dealing with directional data, and we believe it is adequate in our context. Indeed, if in definition (5) we normalize by $\sqrt{|Q|}$ instead of $|Q|$, that is*

$$(6) \quad \mathcal{Q}_1 = \arg \max_{Q \in \mathcal{G}} \text{var} \left(\frac{|\mathbf{G} \wedge Q|}{\sqrt{|Q|}} \right),$$

we obtain a less sparse version of the principal components.

Proposition 5 (Consistency of Principal Components). *Given a stationary and ergodic sequence of random networks $\{\mathbf{G}_t, t \geq 1\}$, the empirical principal components as well as the principal components sets converge a.s. to their corresponding population versions.*

Example 3. Distributions with spherical symmetry satisfy that there does not exist a principal direction, since all directions are equally informative. The distribution given in (4) is one such example. However, a mixture of two or more distributions of that form breaks the symmetry. Here we consider a mixture of 4 exponentials, whose centers are shown in Figure 1 (A), to generate a sample of size 1000. We consider equal costs for each link. The measure is

$$(7) \quad \mu(H) = \mathbb{P}(\mathbf{G} = H) = \sum_{i=1}^4 p_i c_i e^{-\lambda_i d(H, S_i)},$$

where $(p_1, p_2, p_3, p_4) = (0.4, 0.4, 0.1, 0.1)$ and $\lambda_i = 10$ for all i .

The first empirical principal component is the set of three one link networks, E_{12} , E_{13} and E_{14} . The second principal component corresponds to the one link network E_{23} . Figure 1 (B) shows the projection of a sample of size one thousand generated from the exponential model (7). The sample is projected into the first two principal components using the network E_{13} as a representative of the first principal component. We compute the dot products $|G_i \wedge E_{13}|$ and $|G_i \wedge E_{23}|$ for $i = 1, \dots, 1000$. These dot products only take the values 0 or 1 depending on whether the network contains the corresponding link or not. The height in the z-axis

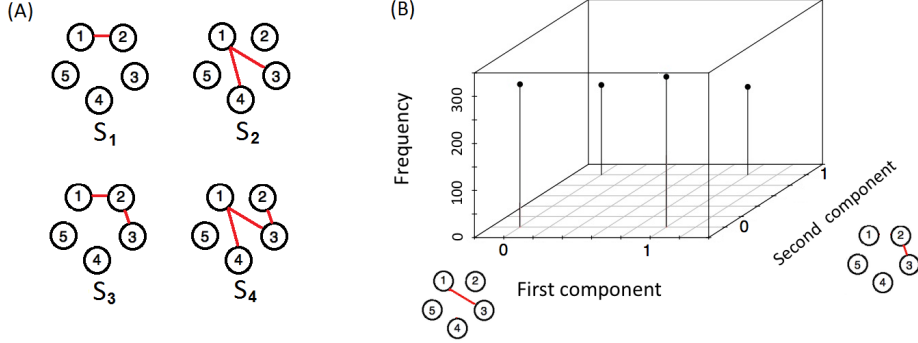


FIGURE 1. (A) Graphs used in the definition of μ . (B) Projected data on the first and second principal components.

shows the number of networks (frequency) in the sample projected at each of the four possibilities.

Both empirical components coincide with the population version. Moreover, we have that $\mu(\mathcal{S}(E_{12})) = \mu(\mathcal{S}(E_{13})) = \mu(\mathcal{S}(E_{14})) = 0.5$ while $\mu(\mathcal{S}(E_{23})) = 0.361$. The proportion of networks in the sample containing $(1, 3)$ is 0.506 while for $(2, 3)$ is 0.378.

6. OTHER MULTIVARIATE TECHNIQUES BASED ON DISTANCES

In this section we briefly discuss some other important multivariate methods. It is clear that extending to our setup other techniques that only rely on distances such as clustering, classification, multidimensional scaling and nonparametric regression is mainly straightforward. The choice of the distance d for this methods is very important. In applications we may be interested in taking into account some “features” of the network to improve the performance of the procedure. A pseudo-metric d_f typically is considered to capture closeness with respect to the selected “features”. These features can be global, such as the diameter or average degree, or can be local, for example the degree of each node. A simple solution to take into account features is to work with the distance

$$\tilde{d} = \alpha d + (1 - \alpha) d_f \quad (\text{for } 0 < \alpha < 1),$$

which is still a metric. Asymptotic results for this distance still hold, while this is not the case if we just use a pseudometric. To illustrate we emphasize two main problems: clustering and classification of networks. The classical k-means algorithm for clustering, as well as k-nearest neighbor, for supervised classification can be applied directly.

6.0.1. Unsupervised classification. Let us suppose that the probability measure μ is such that k groups or clusters of networks can be identified. Two networks in the same group are close together (similar), while networks that belong to different groups are far apart. We want to identify each of the k groups. The most well known clustering methods are k -means or k -medioids, which are only based on the distances between the random elements. More precisely, the algorithm looks for the centers of the groups and then assign each data to its nearest center.

In our setting, what is important is to identify in a good way each of the k center networks, that we denote by $S_1^*, S_2^*, \dots, S_k^*$. The strategy proposed here is the same to that of k-means

(k -medioids in our case). We look the k networks that maximize the depth of order k defined as:

$$D_k(H_1, \dots, H_k) = m - \mathbb{E} \left(\min_{i=1, \dots, k} d(H_i, \mathbf{G}) \right),$$

i.e., we look for subsets $\{S_1^*, \dots, S_k^*\}$ that satisfy

$$D_k(S_1^*, \dots, S_k^*) = \max_{H_1, \dots, H_k} D_k(H_1, \dots, H_k).$$

Then, each network is assigned to its nearest center and we obtain a partition of the space. The asymptotic results for k -means and k -medioids given in Pollard (1981) are valid for compact metric spaces, which covers our setup. In the empirical case we look for the empirical center networks $\hat{S}_1^*, \hat{S}_2^*, \dots, \hat{S}_k^*$ that maximize the empirical depth of order k ,

$$\hat{D}_k(H_1, \dots, H_k) = m - \frac{1}{\ell} \sum_{j=1}^{\ell} \min_{i=1, \dots, k} d(H_i, G_j).$$

6.0.2. Supervised classification. In this case we have a training sample $(\mathbf{Y}_1, \mathbf{G}_1), \dots, (\mathbf{Y}_\ell, \mathbf{G}_\ell)$ where $\{\mathbf{G}_t : t \geq 1\}$ is a sequence of random networks and $\{\mathbf{Y}_t : t \geq 1\}$ stands for the labels that indicates to which subpopulation (group) the individual belongs. For binary classification $\mathbf{Y}_t \in \{0, 1\}$ indicating sick or healthy for instance. The problem consist on predicting the label of a new observation only based on $\mathbf{G}_{\ell+1}$ and the training sample.

The most simple and well known nonparametric classification method is k -nearest neighbors. The method just looks for the k nearest neighbors of $\mathbf{G}_{\ell+1}$ among the sample $\{\mathbf{G}_t : 1 \leq t \leq \ell\}$ and assigns the label by majority vote within the labels of the k -nearest neighbors. It can be applied in our setup as it is just based on distances. The method is asymptotically optimal as long as $k = k(\ell) \rightarrow \infty$ and $k/\ell \rightarrow 0$ as $\ell \rightarrow \infty$ (see for instance Devroye et al., 1996).

7. CASE STUDIES

In this section we apply the results from the previous sections to data from two real networks. We present examples in two categories: networks of level 1 (L1 networks), which corresponds to the case where the data are directly a sequence of networks in time, and networks of level 2 (L2 networks), which are build up from a stochastic process given at each node. For instance, a link between two nodes is present if the correlation between the corresponding stochastic processes of the two nodes is greater than a given threshold. In this case, we lose information while trying to get a simpler model that still retains the relevant characteristics. Level 2 networks are a common tool in functional Magnetic Resonance Imaging (fMRI) studies where they are called functional networks.

7.1. A L1 network example: Social Network. How a disease or information propagates in a population is a very relevant question. For many diseases face-to-face interactions are decisive in the propagation process. Mastrandrea et al. (2015) collected very interesting data to study face-to-face social interaction. By using wearable sensors they were able to describe how do French high school students socially interact (see Mastrandrea et al., 2015, for details). Each of the 327 students involved in the study had a sensor. The sensors exchange packets only when within 1–1.5 meters of one another, thus allowing to know which students are socially interacting in time. The data is publicly available at <http://www.sociopatterns.org/datasets/high-school-contact-and-friendship-networks/>, and corresponds to the face-to-face interactions (links between students) every 20 seconds during five days. For the application shown here we analyze only the last day studied by the

authors (Friday) during all the school day. In the analysis we divide the day in four equal periods, which we label as Morning 1, Morning 2, Afternoon 1 and Afternoon 2. We do not consider the times of “arrival” (8:00–8:30) and “departure” (16:30–17:00) from school, and we assume all costs are equal.

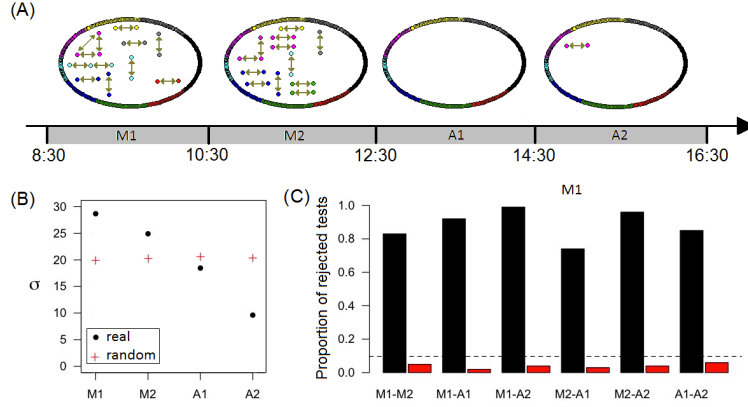


FIGURE 2. (A) Empirical Central Graph and (B) Variability for each of the four time intervals M1, M2, A1, and A2. (C) Proportion of rejected tests, at a significance level of 0.05. The results for a random network are shown in red.

For each time interval of 20 seconds we have a network, obtaining a sequence of 360 networks G_1, G_2, \dots, G_{360} . We compute the empirical Central Graph (Figure 2 (A)) and the Graph Variability σ (Figure 2 (B)) for each sequence. The central networks for the periods M1, M2, A1 and A2 have few links, 12, 11, 0 and 1 respectively. Some of the links that joins two students are present in both M1 and M2 periods (vertical links). Looking at the central networks it seems that the students interact in a different way between the morning and the afternoon.

More precisely, the network variability decreases with time as it is shown in Panel (B). To understand how different are the network probability laws between the time intervals we test it by the random projection procedure described above. One hundred tests were performed, and the proportion of rejected tests (at the level of significance 0.05) is shown in Panel (C) for each pair of periods. In all cases, the proportion of rejected tests is much greater than the critical value (dashed line). The test is able to detect differences even in scenarios where there are few links in comparison with its maximum number (in this case 53301). Namely, the face-to-face interactions are different and this is detected because the law changes along the day.

Next, we compute the central networks, the network variability and the corresponding tests for a sequence of networks generated artificially. More precisely, a link is randomly assigned to one the 1440 time steps, and the same time categories are analyzed. The central network is the null network in the four intervals, and the variability (red crosses in Panel (B)) takes a constant value approximately equal to 20. It is easy to show that this value is the one expected for the Erdős-Renyi model, $\sigma = (1/2 - |p - 1/2|)53301$, for p given by the average density of links in a time step (21.58/53301). Finally, in Panel (C) we show the proportion of rejected tests with red bars (which is clearly below the significance

level) verifying that these randomly “shuffled” networks have the same distribution, as it is expected.

7.2. A L2 network example: Correlation Network. Network techniques based on statistical associations between climate parameters at different points on Earth have been used recently (see for example Donges et al., 2015; Tsonis and Swanson, 2008). Networks are also used to characterize climate dynamics, and phenomena such as the El Niño/Southern Oscillation (Gozolchiani et al., 2008). As far as we know, most results in this area use statistical data to generate a unique network rather than analyzing a *sample* of networks. Here we analyze climate data with the methodology developed in Sections 2-5.

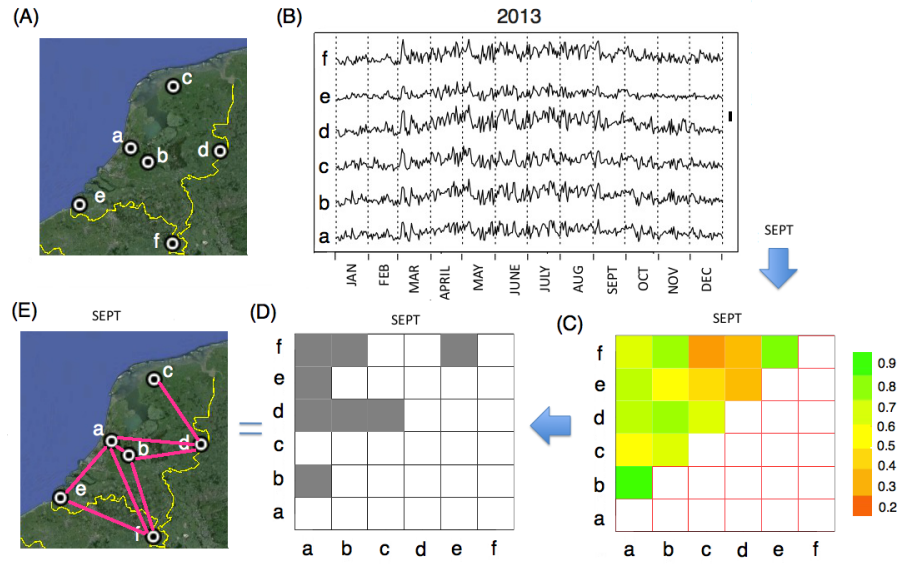


FIGURE 3. (A) Location of the meteorological stations. (B) Thermal amplitude series for the year 2013. The segment on the right end represents 10 degrees Fahrenheit. (C) Correlations between the thermal amplitudes for September 2013. (D) Adjacency matrix obtained using a threshold of 0.48. (E) Associated network.

The data consist on daily thermal amplitude values from six Dutch meteorological stations located across the country (North, North-West, North-East, Middle, West, South-West, South-East). Figure 3 (A) shows the location of each station studied. Figure 3 (B) shows the daily thermal amplitude (temperature range) for each station during the year 2013. For each month we compute the (Spearman) rank correlation matrix between the series, as shown in Figure 3 (C) (by symmetry only the upper values are depicted). We consider rank correlations in order to avoid sensitivity to a few days with extreme values. Finally, a network is obtained by keeping the links with statistically significant correlations, corrected by multiple comparisons (p -values using a t -test for correlations $< 0.05/15$). Two meteorological stations are connected if they share similar thermal behavior. Figure 3 (D) and (E) show the network obtained for September 2013. This method is a standard technique for constructing correlation or functional networks mostly used in Neuroimaging (Bullmore and Sporns, 2009) and Finance (Bonanno et al., 2004).

Using the method described above we construct a network for each month from 1973 to 2013. The data can be obtained at <http://www.ncdc.noaa.gov>. We study the evolution over the last 41 years. Figure 4 (A) shows the central network for each month. The months of March, April, May, June, July, August and September share the same central network which is the complete network. Some of the links connecting geographically distant stations disappear during the coldest months. Moreover, each year the networks observed at each month are different. Figure 4 (B) shows the scale or variability for each month. Low temperature months present networks with more variability. Climate networks for months with colder temperatures (October to February) have in average less links and are more varying.

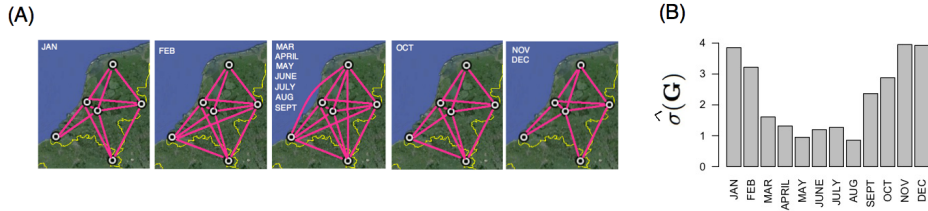


FIGURE 4. (A) Central networks. (B) Scale values.

As a next step, we construct a sequence of networks G_i for the month of May from 1973 to 2013. In Figure 5 (A) the empirical expected depth $(m - \hat{D}(G_i))$ for each year is shown. The month of May was selected because in this month there exists four outlying years (1975, 1984, 1994 and 2012) and the latest has occurred recently. The corresponding networks are shown in Figure 5 (B). All four of them have fewer links than the central network which is complete in this case. In order to understand the outlying behavior, in Panel (C) we show the thermal amplitude time series for the six meteorological stations at two normal years (2011 and 2013) and at the outlying year 2012. It can be observed that in normal years all stations present very similar behavior, however at 2012 the most South-West station at the city of Vlissingen (station e) shows some departure from this general behavior. The thermal amplitude from station e at may of 2012 has a small dependence with the other stations. This last fact generates a climate network with the station e disconnected with the others stations, as it is shown in Panel B (middle network). Probably, the absence of links of station e at may of 2012 is related to particular changes in the air currents from the sea. Vlissingen is the only of the six cities that has a temperate oceanic climate that is milder than the rest of the Netherlands. It is one of the sunniest cities in the Netherlands, and has the lowest rainfall. The other five stations are located at Amsterdam, De Bilt, Leeuwarden, Twente, and Zuid-Limburg and are far (at least 20km) from the sea. Although further analysis is needed to confirm this hypothesis, it seems that the the proximity to the sea can be a plausible scenario for explaining the phenomena observed in May of 2012 at Vlissingen.

Finally, we perform the test proposed in Section 4 to compare two samples of networks. We compare the sample of networks from the month of January with other months. Each sample has a size of 41 (the numbers of years studied). The network distribution from February or December should be very similar to the one from January because an obvious continuity effect. However, when comparing January to June or July marked differences should appear. We tested the null hypothesis of equal distribution between January and each month of the year, i.e. $\mu_{\text{Jan}} = \mu_x$ for each month x using five hundred random projections.

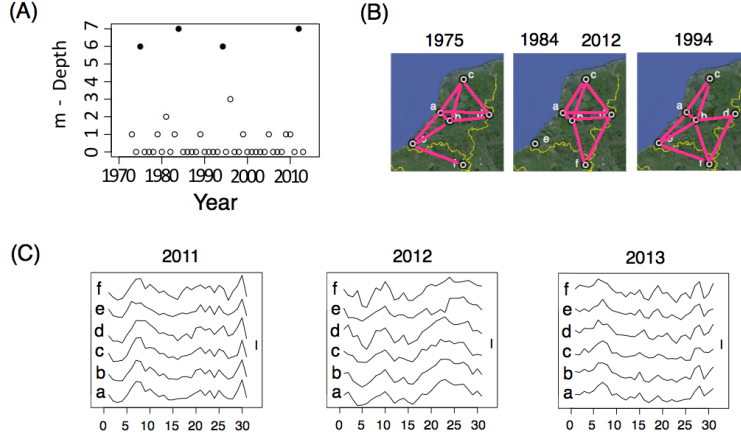


FIGURE 5. (A) Empirical expected distance for each year at the month of May. Black points correspond to outliers. (B) Atypical networks. (C) Thermal amplitude series for the six stations. The segment represents 10 degrees Fahrenheit.

Even with a small sample size the test has an excellent performance. In particular, extremely small p -values were obtained for the months of March through September (see Table 1).

	February	March	April
	0.035	$< 1 \times 10^{-50}$	$< 1 \times 10^{-50}$
May	June	July	August
0	$< 1 \times 10^{-50}$	0	$< 1 \times 10^{-50}$
September	October	November	December
$< 1 \times 10^{-50}$	0.61	0.67	1

TABLE 1. P-values for each of the test comparisons ($H_0 : \mu_G^{\text{Jan}} = \mu_G^x$).

8. DISCUSSION

We propose a general framework to study dynamic random networks with a fixed number of distinguishable nodes. Some classical statistical problems such as clustering and principal component analysis are addressed. All the statistics we define have been constructed using a natural distance between networks and its corresponding L^1 -depth notion. From a theoretical point of view, we believe that the framework we present can be the building block to construct more sophisticated statistical parametric and non parametric models.

One major issue when working with network data is the implementation of theoretical results for large scale networks. While many of the definitions we present involve maximizing over the entire space of networks, we find explicit simple algorithms for the optimization problems which allow to implement our methods for large scale networks and big datasets since the complexity is of order n^2 (linear in the number of possible links).

There are lots of possible applications for the results we present. We analyze two real data examples: the first one corresponds to a face-to-face social interaction network evolving in time, while the second one is an example of the so called correlation networks, for climate data. The results are quite encouraging. It is important to remark that the analysis of correlation networks is becoming a standard procedure in the areas of finance (Bonanno et al., 2004; Aparicio and Fraiman, 2015) and neuroscience (Fraiman et al., 2014, 2009; Bullmore and Sporns, 2009).

Another very important application in Neuroscience is related to the development of new diagnostic methods based on brain network data. This is directly related to the problem of classification of patients (e.g., high or low-risk to have a particular cognitive disorder) for example from their (fMRI, MEG, or EEG) resting state functional networks.

APPENDIX A. PROOFS

A.1. Characterization of the central set.

Proof of Proposition 1. We have that the expected distance from a network H to a random network \mathbf{G} is

$$(8) \quad \mathbb{E}(d(\mathbf{G}, H)) = \sum_{G \in \mathcal{G}} d(G, H) p_G.$$

Let $A(G)$ be the adjacency matrix of the network G and \mathbf{A} the adjacency matrix of the random network \mathbf{G} . Then (8) can be written as

$$\begin{aligned} \sum_{G \in \mathcal{G}} \sum_{i > j} |A(G)_{ij} - A(H)_{ij}| p_G &= \sum_{i > j} \sum_{G \in \mathcal{G}} |A(G)_{ij} - A(H)_{ij}| p_G \\ &= \sum_{i > j} \mathbb{P}(\mathbf{A}_{ij} \neq A(H)_{ij}), \end{aligned}$$

which is minimized by any network H with adjacency matrix $A(H)_{ij} = 1$ if and only if $\mathbb{P}(\mathbf{A}_{ij} = 1) \geq 1/2$. Moreover, if for all i, j

$$(9) \quad \mathbb{P}(\mathbf{A}_{ij} = 1) \neq 1/2,$$

there is a unique network S that minimizes (8) and the adjacency matrix satisfies $A(S)_{ij} = 1$ if and only if $\mathbb{P}(\mathbf{A}_{ij} = 1) > 1/2$.

On the other hand, if condition (9) does not hold, there are many solutions. The maximal center L is the network whose adjacency matrix fulfills $A(L)_{ij} = 1$ when $\mathbb{P}(\mathbf{A}_{ij} = 1) \geq 1/2$ and the set \mathcal{C} contains exactly all subnetworks of L for which S is a subnetwork.

The proof for the empirical version is completely analogous. \square

A.2. Depth determines measure.

Proof of Proposition 2. Let $\mu = (\mu_1, \dots, \mu_M)$ and $\nu = (\nu_1, \dots, \nu_M)$ be two distributions on \mathcal{G} where $M = 2^m$ is the cardinal of the space of networks. For any $H \in \mathcal{G}$, let $d(H) = (d(H_1, H), \dots, d(H_M, H))$. Then, the population depth is

$$D_\mu(H) = m - d(H)^T \mu.$$

Therefore, the depth determines the measure if and only if

$$(10) \quad d(H)^T \mu - d(H)^T \nu = 0 \text{ for all } H \in \mathcal{G} \text{ implies } \mu = \nu.$$

Denote by M the matrix with rows given by $d(H_1), \dots, d(H_M)$. Then (10) is equivalent to $M(\mu - \nu) = 0$, having a unique solution. The result follows from the invertibility of distance matrices. This result was initially proved by Micchelli (1986) and later on by Auer (1995), who provided an elementary proof, that the only uses the triangle inequality. In particular, our metric is just the L^1 distance between the adjacency matrices and the result holds. For the sake of completeness we now state the result in Auer (1995) for distance matrices.

Theorem A. *Let P_1, \dots, P_n be distinct points in \mathbb{R}^k , and $d_{i,j} = \|P_i - P_j\|$. If M_n is the distance matrix with entries $d_{i,j}$, then*

- a) *The $\det M_n$ is positive if n is odd and negative if n is even, in particular M_n is invertible.*
- b) *The matrix M_n has one positive and $n - 1$ negative eigenvalues.*

Applying Theorem A to our setup, we get that the matrix M is invertible. \square

A.3. Characterization of principal components.

Proof of Proposition 3. Note that

$$\text{var} \left(\frac{|\mathbf{G} \wedge \mathbf{Q}|}{|\mathbf{Q}|} \right) = \frac{1}{|\mathbf{Q}|^2} \sum_{G \in \mathcal{G}} \left(\sum_{i>j} c_{ij} A(G)_{ij} A(\mathbf{Q})_{ij} - \sum_{H \in \mathcal{G}} \sum_{i>j} c_{ij} A(H)_{ij} A(\mathbf{Q})_{ij} p_H \right)^2 p_G.$$

We first consider the case when the network \mathbf{Q} has only one link (k, ℓ) , and find within this family the one that maximizes the objective function. Next we prove that for any other network \mathbf{Q} the objective function is bounded by the maximum restricted to the former family. Finally, we show the principal component space is generated by the one link networks.

Let \mathbf{Q} such that $A(\mathbf{Q})_{k\ell} = 1$, and 0 otherwise. Also, let $\mathcal{G}^+ = \{G \in \mathcal{G} : A(G)_{k\ell} = 1\}$ and $\mathcal{G}^- = \{G \in \mathcal{G} : A(G)_{k\ell} = 0\}$. When we search within the one link networks, the objective function reduces to

$$\begin{aligned} \text{var} \left(\frac{|\mathbf{G} \wedge \mathbf{Q}|}{|\mathbf{Q}|} \right) &= \frac{1}{c_{k\ell}^2} \sum_{G \in \mathcal{G}} \left(c_{k\ell} A(G)_{k\ell} - \sum_{H \in \mathcal{G}} c_{k\ell} A(H)_{k\ell} p_H \right)^2 p_G \\ &= \sum_{G \in \mathcal{G}} (A(G)_{k\ell} - \mathbb{P}(\mathbf{A}_{k\ell} = 1))^2 p_G \\ &= \sum_{G \in \mathcal{G}^+} (1 - \mathbb{P}(\mathbf{A}_{k\ell} = 1))^2 p_G + \sum_{G \in \mathcal{G}^-} \mathbb{P}(\mathbf{A}_{k\ell} = 1)^2 p_G \\ &= (1 - \mathbb{P}(\mathbf{A}_{k\ell} = 1))^2 \mathbb{P}(\mathbf{A}_{k\ell} = 1) + \mathbb{P}(\mathbf{A}_{k\ell} = 1)^2 \mathbb{P}(\mathbf{A}_{k\ell} = 0) \\ &= \mathbb{P}(\mathbf{A}_{k\ell} = 1) (1 - \mathbb{P}(\mathbf{A}_{k\ell} = 1)), \end{aligned}$$

and the solution is the one link graph for which $\mathbb{P}(\mathbf{A}_{k\ell} = 1)$ is closest to $1/2$.

In the general case, we want to find \mathbf{Q} that maximizes

$$\begin{aligned} \text{var} \left(\frac{|\mathbf{G} \wedge \mathbf{Q}|}{|\mathbf{Q}|} \right) &= \frac{1}{|\mathbf{Q}|^2} \sum_{G \in \mathcal{G}} \left(\sum_{(i,j) \in \mathbf{Q}} c_{ij} A(G)_{ij} - \sum_{H \in \mathcal{G}} \sum_{(i,j) \in \mathbf{Q}} c_{ij} A(H)_{ij} p_H \right)^2 p_G \\ &= \sum_{G \in \mathcal{G}} \sum_{(i,j) \in \mathbf{Q}} w_{ij} (A(G)_{ij} - \mathbb{P}(\mathbf{A}_{ij} = 1))^2 p_G, \end{aligned}$$

where $w_{ij} = c_{ij} / \sum_{(p,q) \in Q} c_{pq}$. Now, since the weights w_{ij} add to one, we have

$$\begin{aligned} \text{var} \left(\frac{|\mathbf{G} \wedge \mathcal{Q}|}{|\mathcal{Q}|} \right) &\leq \sum_{(i,j) \in Q} w_{ij} \max_{(i,j)} \mathbb{P}(\mathbf{A}_{ij} = 1) (1 - \mathbb{P}(\mathbf{A}_{ij} = 1)) \\ &= \max_{(i,j)} \mathbb{P}(\mathbf{A}_{ij} = 1) (1 - \mathbb{P}(\mathbf{A}_{ij} = 1)), \end{aligned}$$

which corresponds to the one link optimum. \square

A.4. Consistency of Principal Components.

Proof of Proposition 4. For each $Q \in \mathcal{G}$ from the Ergodic Theorem we have the following.

$$\text{a) } \Lambda_\ell(Q) = \frac{1}{\ell} \sum_{k=1}^{\ell} |G_k \wedge Q| \rightarrow \mathbb{E}(|\mathbf{G} \wedge Q|), \text{ almost surely as } \ell \rightarrow \infty.$$

$$\begin{aligned} \text{b) } \Delta_\ell(Q) &= \widehat{\text{var}} \left(\frac{|\mathbf{G} \wedge Q|}{Q} \right) \\ &= \frac{1}{\ell} \sum_{k=1}^{\ell} \left(\frac{|G_k \wedge Q| - \Lambda_\ell(Q)}{|\mathcal{Q}|} \right)^2 \\ &= \frac{1}{\ell} \sum_{k=1}^{\ell} \frac{|G_k \wedge Q|^2}{|\mathcal{Q}|^2} + \frac{\Delta_\ell^2(Q)}{|\mathcal{Q}|^2} - \frac{2}{\ell} \sum_{k=1}^{\ell} \frac{|G_k \wedge Q|}{|\mathcal{Q}|^2} \Lambda_\ell(Q), \end{aligned}$$

which converges almost surely to

$$(11) \quad \mathbb{E} \left(\frac{|\mathbf{G} \wedge Q|^2}{|\mathcal{Q}|^2} \right) + \mathbb{E} \left(\frac{|\mathbf{G} \wedge Q|}{|\mathcal{Q}|^2} \right)^2 - 2\mathbb{E} \left(\frac{|\mathbf{G} \wedge Q|}{|\mathcal{Q}|^2} \right)^2 = \text{var} \left(\frac{|\mathbf{G} \wedge Q|}{|\mathcal{Q}|} \right).$$

c) Since the space \mathcal{G} is finite (11) entails that $\hat{\mathcal{Q}}_1 \rightarrow \mathcal{Q}_1$ almost surely, i.e., $\hat{\mathcal{Q}}_1 = \mathcal{Q}_1$ for ℓ large enough almost surely, which entails that the principal components converge because the geodesics will coincide eventually.

For the next principal component the proof is analogous. \square

A.5. Convergence of empirical depth.

Proof of Theorem 2. From the Ergodic Theorem we have that $\hat{D}_\ell(H) \rightarrow D(H)$ almost surely as $\ell \rightarrow \infty$ for each $H \in \mathcal{G}$. Since \mathcal{G} is finite we get uniform convergence. \square

Proof of Theorem 3. Recall that a sequence of random elements $\mathbf{X} := (\mathbf{X}_t, t \geq 1)$ is a strong mixing sequence if it fulfills the following condition. For $1 \leq j < \ell \leq \infty$, let \mathcal{F}_j^ℓ denote the σ -field of events generated by the random elements X_k , $j \leq k \leq \ell$ ($k \in \mathbf{N}$). For any two σ -fields \mathcal{A} and \mathcal{B} , define

$$\alpha(\mathcal{A}, \mathcal{B}) := \sup_{A \in \mathcal{A}, B \in \mathcal{B}} |\mathbb{P}(A \cap B) - \mathbb{P}(A)\mathbb{P}(B)|.$$

For the given random sequence \mathbf{X} , for any positive integer n , define the dependence coefficient

$$\alpha(n) = \alpha(\mathbf{X}, n) := \sup_{j \geq 1} \alpha(\mathcal{F}_1^j, \mathcal{F}_{j+n}^\infty).$$

The random sequence \mathbf{X} is said to be “strongly mixing”, or “ α -mixing”, if $\alpha(n) \rightarrow 0$ as $n \rightarrow \infty$. This condition was introduced by Rosenblatt (1956). By assumption, we have that the sequence of random networks $\{\mathbf{G}_t : t \geq 1\}$ is a strongly mixing sequence. In order to prove the theorem we use the following result (see for instance Peligrad, 1986).

Theorem B. Let $\{\mathbf{X}_t : t \geq 1\}$ be a strictly stationary centered α -mixing sequence, and let $\mathbf{S}_\ell = \sum_{t=1}^\ell \mathbf{X}_t$. Assume that for some $C > 0$

$$|\mathbf{X}_1| < C \text{ almost surely, and } \sum_{n=1}^{\infty} \alpha(n) < \infty.$$

Then,

$$\sigma^2 := \mathbb{E}(\mathbf{X}_1^2) + 2 \sum_{k=2}^{\infty} \mathbb{E}(\mathbf{X}_1 \mathbf{X}_k),$$

is absolutely summable. If in addition $\sigma^2 > 0$, then $\mathbf{S}_\ell / \sqrt{\ell} \sigma$ converges weakly to a standard normal distribution.

First observe that

$$\beta^T \mathbf{Z}_\ell = \frac{1}{\ell} \sum_{k=1}^{\ell} \mathbf{W}_k, \quad \text{with} \quad \mathbf{W}_k = \sum_{j=1}^{2^m} \beta_j (d(H_j, \mathbf{G}_k) - \mathbb{E}(d(H_j, \mathbf{G}_1))),$$

where $\{\mathbf{W}_t : t \geq 1\}$ is a strictly stationary, bounded, centered α -mixing sequence, fulfilling $\sum_{n=1}^{\infty} \alpha(n) < \infty$. On the other hand, we have that

$$\mathbb{E}(\mathbf{W}_1^2) = \beta^T \mathbb{E}(\mathbf{Y}_1^T \mathbf{Y}_1) \beta \text{ and } \mathbb{E}(\mathbf{W}_1 \mathbf{W}_k) = \beta^T \mathbb{E}(\mathbf{Y}_1^T \mathbf{Y}_k) \beta,$$

and the result follows from Theorem B. \square

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